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Material Strength at High Pressure

LDRD Strategic Initiative

Final Report

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1.0 Summary

Various aspects of the Laboratory's national security mission are now highly dependent on accurate computer code simulations of plastic flow (i.e., non-reversible deformation) of materials under conditions of high hydrostatic pressure. Strength models are typically dependent on pressure, temperature, and strain rate. Current strength models can not be extrapolated to high pressure because they are not based on the underlying mechanisms of plastic deformation.

The critical need for predictive models of material strength, which describe flow stress in computer code simulations, has motivated LLNL's multiscale modeling efforts. Over the past three years, the "Material Strength at High Pressure" LDRD Strategic Initiative has established a framework for the development of predictive strength models for deformation of metals under conditions of high hydrostatic pressure. Deformation experiments have been developed to measure the effect of high pressure on the yield strength and work hardening behavior of high purity Mo and Ta single crystals. The over arching goal of the SI is to experimentally validate multiscale-modeling capabilities for deformation of metals under conditions of high pressure. The work performed and accomplished is a necessary next step in the development of predictive strength models.

Our initial experimental results show that the influence of pressure is to dramatically increase the work hardening rate of Ta. Bridgman also observed this in experiments performed in the 1950's. Currently there is very little modern data on this phenomena, or theoretical understanding. The work started by this SI is a first step in a comprehensive understanding of plasticity under conditions of high pressure and we expect eventually to be able to incorporate the proper physics into dislocation dynamics (DD) simulations to capture the increase in work hardening that we observe experimentally.

In the following sections we briefly describe the work that was performed in the areas of theory and DD simulation development (Section 2) and experimental work (Section 3). Journal articles and technical reports, which are essentially drafts of papers that will be submitted, are attached to this final report.

2.0 Simulations of High Pressure and Strain Rate Deformation

Multiscale modeling is based on information passing, where results of simulations at small length scales (e.g., dislocation mobility) are used in simulations of plastic deformation performed at higher length scales. The principal mechanism by which plastic deformation in metals occurs is the generation and motion of dislocations (line defects) in the crystal lattice. The primary goal of LLNL's multiscale modeling effort is to account for the unit mechanisms associated with dislocation motion, multiplication, and interaction in strength models used in computer code simulations. DD simulations form the critical link that allows information generated at the atomistic length scale to be utilized in continuum computer code simulations.

2.1 Massively-Parallel Dislocation Dynamics Simulations

In the year 2000 it was clear that a significant leap in the efficiency of current dislocation dynamics simulations was required to render them useful for the prediction of strength properties at high pressures, strain rates, and large extents of plastic strain. To this end, the "Material Strength at High Pressure" SI focused on the development of a new all-parallel DD code designed from the ground up to run on ASCI massively parallel machines. The following paper describes the new code and it applications.

Massively-Parallel Dislocation Dynamics Simulations,

Wei Cai, Vasily Bulatov, Tim Pierce, Masato Hiratani, Moono Rhee, Maria Bartelt and Meijie Tang,

UCRL-JC-153525

2.2 Dislocation Mobility at High Pressure and Velocity

Although the fundamental nature of plastic deformation of metals under high pressure is similar to that at low pressure (i.e., generation, motion, and interaction of dislocations), these unit mechanisms can be substantially different under high-pressure/high-strain-rate conditions. For example, a simulation of dislocation generation under low and high stress levels can lead to different multiplication rates and dislocation configurations. Another example of mobility phenomena unique to high-strain-rate deformation is the non-conservative nature of dislocation motion at very high dislocation velocities. Under low-pressure, strain-rate deformation conditions, dislocations glide though the lattice with little or no generation of defects. However, at high strain rates, the rapidly moving dislocation can leave debris in the form of point defects and dislocation loops. The following papers describe some of the work associated with dislocation mobility under high pressure and strain rate conditions that was produced under this SI.

Atomistic Simulation of Defect Properties in BCC Tantalum,

Lin H. Yang, Per Soderlind and John A. Moriarty,

UCRL-JC-148128

Atomistic Simulations of Dislocations and Defects,

John A, Moriarty, Vaclav Vitek, Vasily bulatov and Sidney yip,

UCRL-JC-152885

Mobility Laws in Dislocation Dynamics Simulations,

Wei Cai and Vasily Bulatov,

UCRL-JRNL-200968

Dynamic Transitions from Smooth to Rough to Twinning in Dislocation Motion

Jaime Marian, Wei Cai and Vasily V. Bulatov

UCRL-JRNL-202502

The physics of dislocation mobility currently used in dislocation dynamics are still in need of development, however, the utility of using dislocation dynamics simulations to develop data bases of information for higher length-scale models has been demonstrated. The following paper describes the first development in statistical information on dislocation density and character generated by a series of DD simulations that were subsequently used to develop constants for an advanced continuum crystal plasticity model:

Simulations on the Growth of Dislocation Density During Stage "0" Deformation in BCC Metals,

Athanosios Arsenlis and Meijie Tang,

UCRL-JC-149994

3.0 Experimental Techniques

Experimental techniques were developed specifically to validate dislocation dynamics simulations of high-pressure, high-strain-rate deformation. The study materials were purified molybdenum and tantalum single crystals, which are prototypical bcc metals and are of particular interest to various Laboratory programs. We focused on the development of three experiments:

- Diamond anvil cell (DAC)
- Bridgman Cell (Tri-anvil)
- Weak-shock wave-profiles

Each of these experiments was specifically chosen to validate dislocation behavior in the various ranges of pressure and dislocation-velocity, and associated physics issues. All of the experiments were successfully developed under the SI funding and initial data shows that deformation under high pressure results in work hardening that is much higher than expected. Ultimately this data will be indispensable in future DD validation efforts because there is little on no previous data that has the fidelity with respect to yield and slip system activity of bcc single crystals.

3.1 DAC Controlled Deformation Experiments

A DAC experiment to determine the strength properties of single crystals over a range of pressures (100–700 kbar) and strain-rates ($10–10^{-5}$ s^{-1}) was developed to determine the yield and work hardening behavior of Mo single crystals. The unique aspect of the new DAC experiment is that it allows a test sample to be pressurized prior to applying additional axial load. Thus, very accurate determinations of the shear stress required to activate plastic flow can be determined at precise values of hydrostatic pressure. The following paper, which will subsequently be submitted for publication, described the DAC experiment and contains preliminary information on the strength of high-purity [001] Mo single crystals:

Deformation of Single Crystal Molybdenum at High Pressure,

Brian P. Bonner[1], Chantel Aracne[1], Daniel L. Farber[1], Carl O. Boro[1], David Lassila[2]

UCRL-TR-202579

Ultimately the interpretation of DAC deformation experiments will involve simulations (both DD and continuum plasticity). One of the most important aspects of the simulations will be the diamond/Mo boundary condition, i.e. the friction associated with the Mo test sample as it deforms against the diamond anvil.

Determination of the Coefficient of Friction Between Metal and Diamond Under High Hydrostatic Pressure,

J. C. Crowhurst, I. M. Darnell, A. F. Goncharov, D. H. Lassila, J. M. Zaug,

UCRL-JRNL-202370

3.2 "Tri-Anvil" Bridgman Cell Crystal Plasticity Experiments

A new procedure to study the mechanical properties of materials deformed by shearing strains while maintained under high pressure has been described. The paper focuses on the details of the experiment and qualitatively in the changes experienced by the specimens subjected to high pressures.

In order to use this procedure to study the properties of the mainly as a result of shear stresses, materials such as the dislocation mobility of single crystals, is desirable that the hydrostatic pressure contributes, in no way in the ideal case, or at least not in a significant level before the shear process. Based on the results exposed here, this procedure has proven to be a good method to study these properties. Although the optical microscopy analysis showed that the specimens maintained the deformed shape after unloading. The microstructure seems not to change due solely to the effect of the pressure applied. This was corroborated via Vickers characterization, with the hardness

being almost equal to the un-deformed material. This was also validated through the EBSD and TEM imaging, with neither technique showing significant deformation of the microstructure nor dislocation multiplication.

Also the experiment allows the validation of models for materials held under high pressure. The Steinberg-Guinan model was tested using polycrystalline Ta. The outcome of these tests showed that hydrostatic pressure plays a more influent role than expected on properties such as yield strength, showing that it increases more rapidly than that predicted by available models.

Measurement of Shear Strength in BCC materials Subjected to Moderate Pressures,

J.P. Escobedo[1], D.P. Field[1], D.H. Lassila[2], M.M. Leblanc[2], and B.P. Bonner[2]

UCRL-TR-202509

3.3 Investigation of Plasticity in the Phonon Drag Regime

Dynamically loaded gas gun experiments were performed to validate the predictive capabilities of 3-D dislocation dynamics (DD) code simulations at very high strain rates and dislocation velocities where the phonon drag mechanism will be dominant. The experiments were performed in the weak-shock regime on high-purity Ta single crystals with [001] compression axes. We have also performed shock-recovery experiments and are in the process of analyzing the dislocation structure generated by weak-shocks using transmission electron microscopy (TEM). Together the weak-shock wave profiles and TEM results will be used to validate the dislocation structure predicted by the DD simulations. DD simulation results are presented to demonstrate the feasibility of using a combined experimental/simulation effort for the validation of dislocation generation and mobility physics issues in the phonon drag regime.

Weak-Shock Wave Profiles for Validation of 3-D Dislocation Dynamics Simulations,

David H. Lassila and James U. Cazamias
UCRL-TR-202511

3.4 Transmission Electron Microscopy Experiments

Initial dislocation structures in as-annealed high-purity Mo single crystals, and deformation substructures of the crystals compressed at room temperature under different strain rates have been examined and studied in order to elucidate the physical mechanisms of dislocation multiplication and motion in the early stages of plastic deformation. The initial dislocation density was measured to be in a range of $10^6 \sim 10^7$ cm^{-2}. More importantly numerous grown-in super jogs were observed along screw dislocation lines. After testing in compression, dislocation density (mainly screw

dislocations) increased to $10^7 \sim 10^8$ cm^{-2}. Besides, the formation of dislocation dipoles (debris) due to the nonconservative motion of jogged screw dislocations was found to be dependent of the strain rates. While little dislocation dipoles (debris) were found in the crystal tested quasi-statically (10^{-3} s^{-1}), more cusps along screw dislocation lines and numerous dislocation dipoles (debris) were observed in the crystal compressed under the strain rate of 1 s^{-1}. Physical mechanisms for dislocation multiplication as well as dipole formation from jogged screw dislocations under different strain rate conditions are accordingly proposed and discussed.

Initial Dislocation Structure and Dynamic Dislocation Multiplication in Mo single crystals,

L. M. Hsiung and D. H. Lassila,

UCRL-JC-138788

3.5 Quantification of Crystal Plasticity

The validation of dislocation dynamics simulation can involve comparison to a minimal amount of experimental information, for example simply a uniaxial measurement of plastic yield and/or work hardening rate. However, these types of zero'th order validation do not provide for uniqueness. For example, a multitude of combinations of slip system activities may result in the same "uniaxial" work hardening. The Material Strength at High Pressure SI work is therefore somewhat dependent on the development of a more sophisticated methodology for validation. A paper, which was published in 2003, outlines a detailed experimental method for the determination of slip-system activity and servers as essentially a bar for future validation efforts.

Single Crystal Deformation Experiments for Validation of Dislocation Dynamics,

D. H. Lassila, Mary M. LeBlanc and Moono Rhee

UCRL-CONF-200935

3.6 Phonon Dispersions and Elastic Constants of Mo Single Crystal at High Pressure

Inelastic x-ray scattering experiments under hydrostatic pressure provide insight into the nature of materials under extreme conditions by determining how normal modes of the crystal lattice change with atomic spacing. Molybdenum exhibits a giant Kohn anomaly or mode softening at high phonon momentum that has not been studied at pressure because of the inherent limitations of neutron scattering methods. It also is a good representative of BCC metals, and as such provides a means for understanding that important metal class. The initial slope of the phonon dispersion relation determines the elastic modulus for each mode.

X-ray scattering measurements were done on single crystals with micron dimensions in

a Diamond Anvil Cell to pressures of 37 GPa at beam line ID-28 at the ESRF. The complete phonon dispersion curves were determined. Elastic moduli calculated from the initial slopes were compared to first principles calculations of the pressure dependent moduli computed by the MGPT method (Moriarity et al, 2004). Agreement is excellent with experimental error. Understanding the details of phonon dispersion at higher momentum provide the most stringent test of first principles methods and will be undertaken in future calculations.

The following individuals were involved in this work and are currently preparing a manuscript for submission to an archival journal:

Daniel L. Farber[1], M. Krisch[2],Chantel Aracne[1], F. Occelli[1], D. Antonangeli[2]

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European Synchrotron Radiation Laboratory, Grenoble, France[2]

4.0 Conclusions

Our initial experimental results show that the influence of pressure is to dramatically increase the work hardening rate of Ta, which is consistent with Bridgman's observations in the 1950's. Currently there is very little modern data on this phenomena, or theoretical understanding. The controlled DAC deformation experiments and Bridgman "tri-anvil experiments are beginning to establishing a modern data base on the effects of high pressure on the yield and work hardening behavior of bcc metals. The new will provide critical data for development a comprehensive understanding of plasticity under conditions of high pressure and we expect eventually to be able to incorporate the proper physics into DD simulations to capture the increase in work hardening that we observe experimentally.

The use of weak-shock wave profiles has been employed since the mid '60's to study plasticity at high strain rates and moderate pressure, but the major limitation in fundamental understanding has been our ability to model the experiment. Recently the use of DD simulations to model weak-shocks has been demonstrated by Zbib and others and thus we now have a way to model the fundamental dislocation behavior associated with weak shock propagation in single crystals. Under this SI we have performed weak-shock experiments on Ta single crystals (wave profiles and recovery of shocked materials. Together the DD simulation capability to model weak-shock propagation and the experimental data will provide a break through in our understanding of plasticity at strain rates on the order of $10^5 – 10^6$ s-1.

While there is still a lack of detailed validation of DD simulations with regard to slip system activity, the simulation capabilities developed under this SI have demonstrated the viability of using this class of simulation to link atomistic information to continuum crystal plasticity theory and models. Both large plastic strains and dislocation densities

can be simulated using the new all-parallel DD code designed from the ground up to run on ASCI massively parallel machines.

Many physics issues or "unit processes" associated with dislocation mobility and dislocation-dislocation interaction have been examined and published under the SI work plan. For example, the effect of high pressure on the Peierls barrier, kink nucleation at junctions, and non-conservative motion at high dislocation velocities. While some of this information has been incorporated into DD simulation, much more still needs to be done.

Capturing the correct physics associated with the experimentally observed increase in work hardening behavior under conditions of high pressure is possible using DD simulations because of the significant progress in both development of the all-parallel DD simulation codes and progress in atomistic simulations of dislocation phenomena. Deformation experiments specifically designed to quantify yield and work hardening behavior of bcc single crystals under conditions of high pressure have been successful. In this regard, the work under this SI has made significant progress toward attainment of the over arching goal of a experimentally validated capability DD simulation to simulate deformation of bcc metal under conditions of high pressure.

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